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Time Evolution of Density Matrices Using BBGKY Hierarchy
ALI AKBARI, Nano-Bio Spectroscopy Group, Departamento de Física de Materiales, Universidad del País Vasco, San Sebastián, Spain, JAVAD HASHEMI, RISTO NIEMINEN, Department of Applied Physics, Aalto University, P.O. Box 11100, FI-00076 AALTO, Finland, ROBERT VAN LEEUWEN, Department of Physics, Nanoscience Center, FIN 40014, University of Jyväskylä, Jyväskylä, Finland, ANGEL RUBIO, Nano-Bio Spectroscopy Group, Departamento de Física de Materiales, Universidad del País Vasco, San Sebastián, Spain — Our work starts with the BBGKY hierarchy equations which can be straightforwardly derived from the time-dependent Schrödinger equation for each n-body reduced density matrices (n-RDM). The equations of the BBGKY hierarchy in each level, couple an n-RDM to the $(n+1)$-RDM. In order to make this set of equations tractable we need to truncate the hierarchy. While people usually truncate the hierarchy at the first level, one can also truncate it at the level of second equation by approximating 3-RDM in terms of 2-RDM and 1-RDM. Regardless of approximations that we choose, the total energy and momentum will be conserved if we solve the first and second equation together. However, we will show that most of the existing approximations are unstable and even diverging in time and ponder the reasons behind it.

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